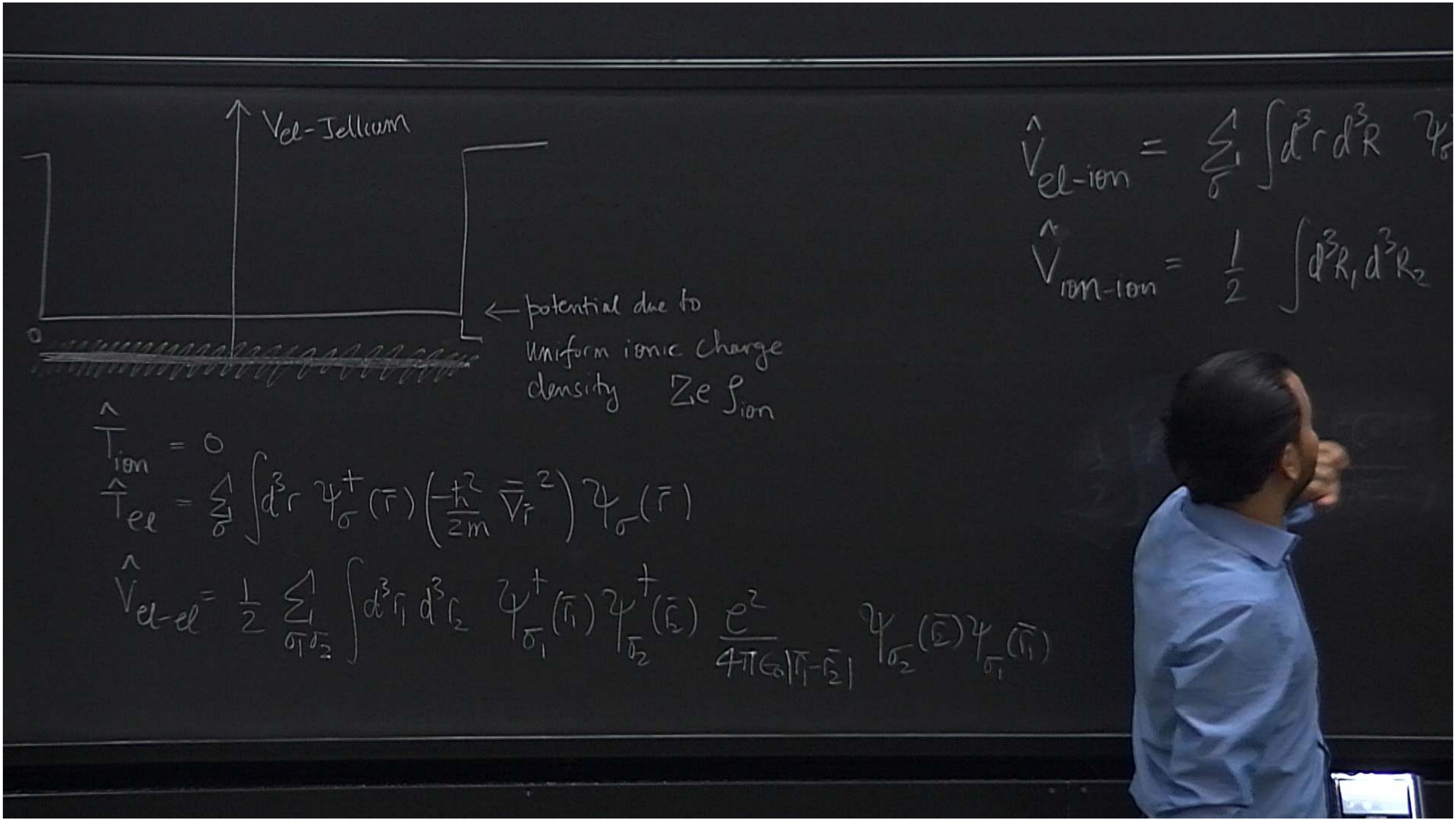
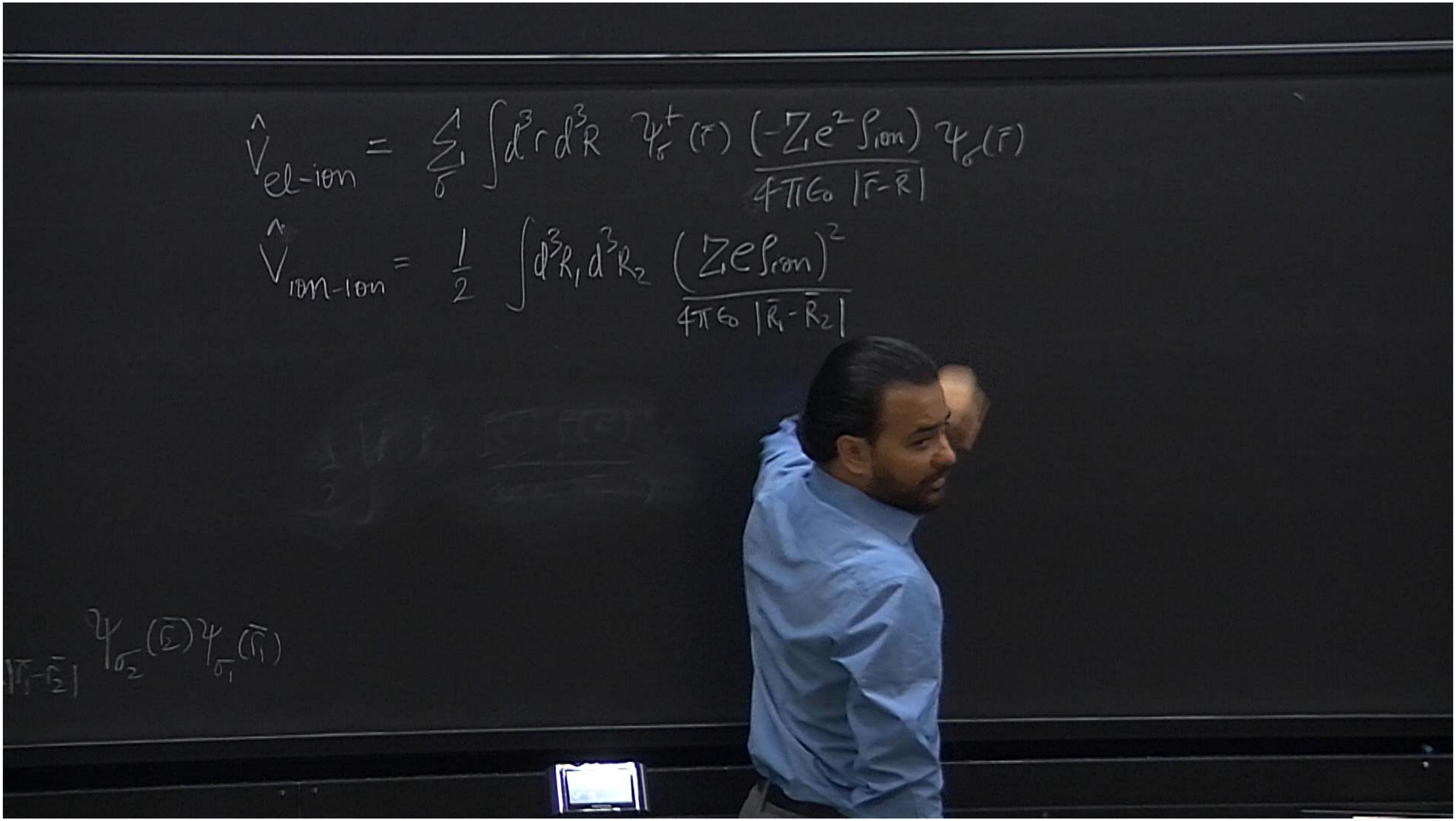
Title: PSI 17/18 - Condensed Matter - Lecture 6

Date: Nov 13, 2017 10:45 AM

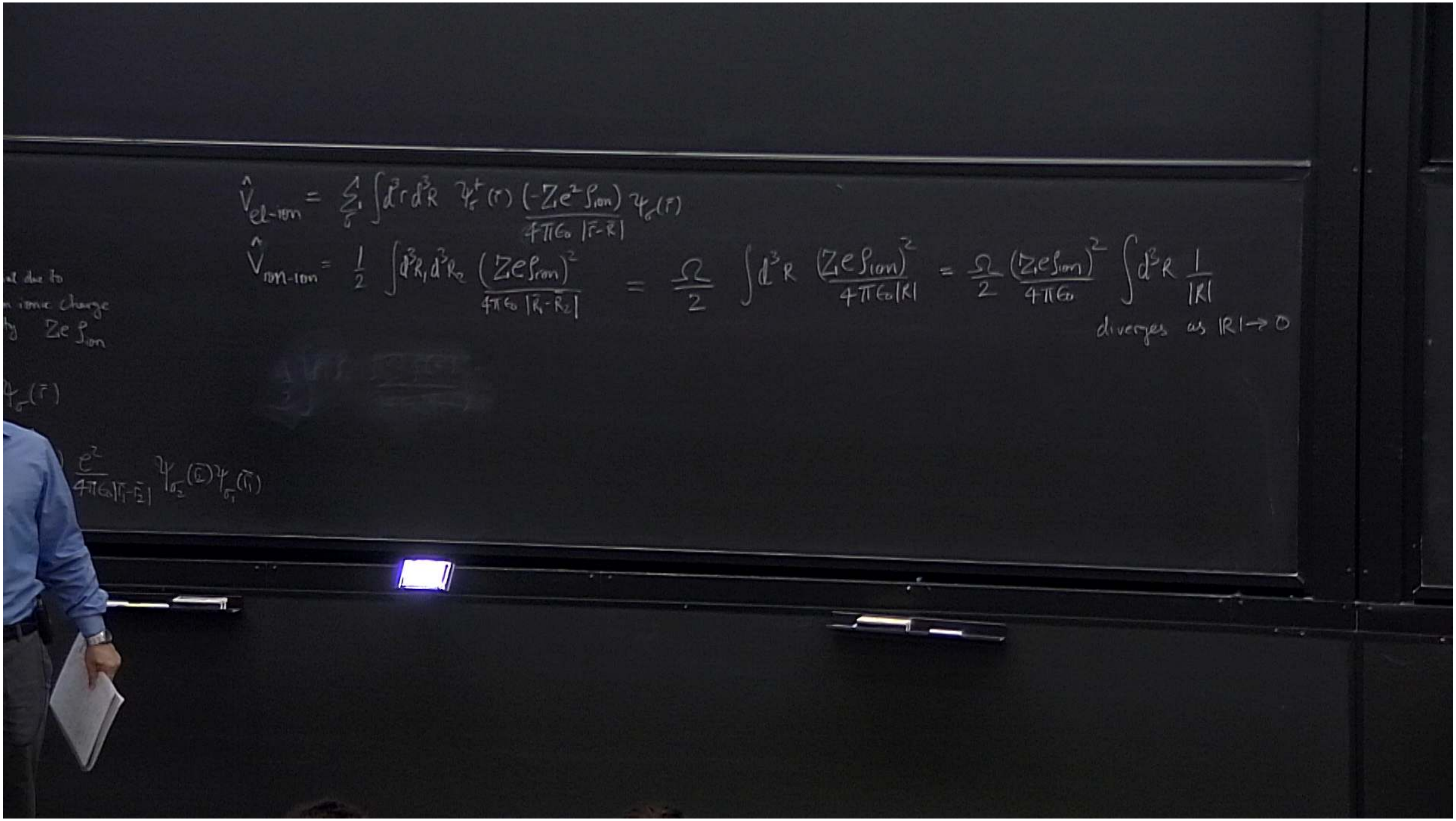
URL: http://pirsa.org/17110031

Abstract:


$V_{el\text{-}Jellium}$
0
← potential due to uniform ionic charge density $Ze\rho_{ion}$
$\hat{T}_{ion} = 0$
$\hat{T}_{el} = \sum_\sigma \int d^3r\, \psi^\dagger_\sigma(\bar{r}) \left(-\frac{\hbar^2}{2m} \bar{\nabla}_r^2\right) \psi_\sigma(\bar{r})$
$\hat{V}_{el\text{-}el} = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3r_1\, d^3r_2\, \psi^\dagger_{\sigma_1}(\bar{r}_1) \psi^\dagger_{\sigma_2}(\bar{r}_2) \frac{e^2}{4\pi\epsilon_0 |\bar{r}_1 - \bar{r}_2|} \psi_{\sigma_2}(\bar{r}_2) \psi_{\sigma_1}(\bar{r}_1)$
$\hat{V}_{el\text{-}ion} = \sum_\sigma \int d^3r\, d^3R\ \psi^\dagger_\sigma$
$\hat{V}_{ion\text{-}ion} = \frac{1}{2} \int d^3R_1\, d^3R_2$



$\hat{V}_{el-ion} = \sum_{\sigma} \int d^3r\, d^3R\ \psi_\sigma^{+}(\bar{r}) \frac{(-Z e^2 \rho_{ion})}{4\pi\epsilon_0 |\bar{r}-\bar{R}|} \psi_\sigma(\bar{r})$
$\hat{V}_{ion-ion} = \frac{1}{2} \int d^3R_1\, d^3R_2 \frac{(Z e \rho_{ion})^2}{4\pi\epsilon_0 |\bar{R}_1-\bar{R}_2|}$
$|\bar{r}_1-\bar{r}_2|\ \psi_{\sigma_2}(\bar{r}_2)\psi_{\sigma_1}(\bar{r}_1)$



$\hat{V}_{el-ion} = \sum_{\sigma} \int d^3r\, d^3R\; \psi_{\sigma}^{\dagger}(\bar{r})\, \frac{(-Z_i e^2 \rho_{ion})}{4\pi\epsilon_0\, |\bar{r}-\bar{R}|}\, \psi_{\sigma}(\bar{r})$
$\hat{V}_{ion-ion} = \frac{1}{2} \int d^3R_1\, d^3R_2\, \frac{(Ze\rho_{ion})^2}{4\pi\epsilon_0\, |\bar{R}_1-\bar{R}_2|} = \frac{\Omega}{2} \int d^3R\, \frac{(Ze\rho_{ion})^2}{4\pi\epsilon_0 |R|} = \frac{\Omega}{2} \frac{(Z_i e \rho_{ion})^2}{4\pi\epsilon_0} \int d^3R\, \frac{1}{|R|}$
diverges as $|R| \to 0$
al due to
n ionic charge
ty $Ze\rho_{ion}$
$\psi_{\sigma}(\bar{r})$
$\frac{e^2}{4\pi\epsilon_0|\bar{r}_1-\bar{r}_2|}\psi_{\sigma_2}(\bar{r}_2)\psi_{\sigma_1}(\bar{r}_1)$

$$\frac{\ldots \rho_{ion})}{|\bar{r}-\bar{R}|} \psi_\sigma(\bar{r})$$

$$= \frac{\Omega}{2} \int d^3R \, \frac{(Z_1 e \rho_{ion})^2}{4\pi\epsilon_0 |R|} = \frac{\Omega}{2} \left(\frac{Z_1 e \rho_{ion}}{4\pi\epsilon_0}\right)^2 \int d^3R \, \frac{1}{|R|}$$

diverges as $|R| \to 0$

$(\bar{r})$

$$\frac{\Omega}{2}\int d^3R \left(\frac{Z_i e \rho_{ion}}{4\pi\epsilon_0 |R|}\right)^2 = \frac{\Omega}{2}\left(\frac{Z_i e \rho_{ion}}{4\pi\epsilon_0}\right)^2 \int d^3R \, \frac{1}{|R|}$$

diverges as $|R| \to 0$

$$\left\langle \sum_{\sigma} \psi_\sigma^\dagger(\bar{r})\, \psi_\sigma(\bar{r}) \right\rangle$$

$$= \sum_\sigma \int d^3r\, d^3R\; \psi_\sigma^\dagger(\bar r)\, \frac{\left(-Z e^2 \rho_{ion}\right)}{4\pi\epsilon_0\, |\bar r - \bar R|}\, \psi_\sigma(\bar r)$$

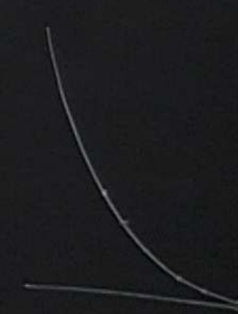
$$= \frac{1}{2} \int d^3R_1\, d^3R_2\, \frac{\left(Z e \rho_{ion}\right)^2}{4\pi\epsilon_0\, |\bar R_1 - \bar R_2|} = \frac{\Omega}{2} \int d^3R\, \frac{\left(Z e \rho_{ion}\right)^2}{4\pi\epsilon_0 |R|} = \frac{\Omega}{2} \frac{\left(Z e \rho_{ion}\right)^2}{4\pi\epsilon_0}$$

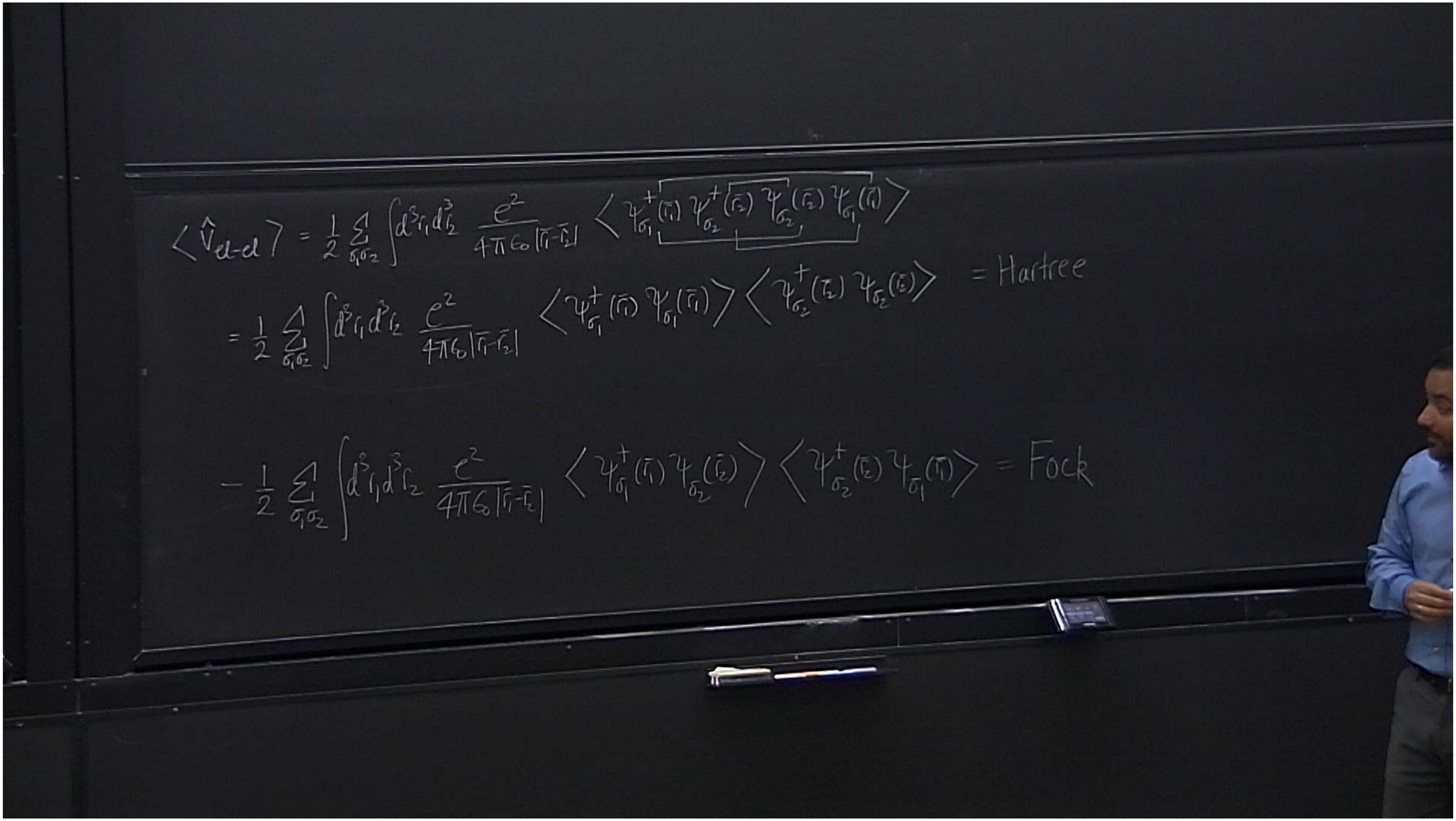
dive

$$\langle \hat V_{el\text{-}ion} \rangle = \int d^3r\, d^3R\, \frac{\left(-Z e^2 \rho_{ion}\right)}{4\pi\, \epsilon_0\, |\bar r - \bar R|} \underbrace{\left\langle \sum_\sigma \psi_\sigma^\dagger(\bar r)\, \psi_\sigma(\bar r) \right\rangle}_{= \rho_{el}}$$

$$= -\Omega\, \frac{Z e^2 \rho_{ion}\, \rho_{el}}{4\pi\epsilon_0} \int d^3R\, \frac{1}{|R|}$$

diverges as $|R| \to 0$




$\langle \hat{V}_{el\text{-}el} \rangle = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 d^3 r_2 \frac{e^2}{4\pi\epsilon_0 |\bar{r}_1 - \bar{r}_2|} \langle \psi^+_{\sigma_1}(\bar{r}_1) \psi^+_{\sigma_2}(\bar{r}_2) \psi_{\sigma_2}(\bar{r}_2) \psi_{\sigma_1}(\bar{r}_1) \rangle$
$= \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 d^3 r_2 \frac{e^2}{4\pi\epsilon_0 |\bar{r}_1 - \bar{r}_2|} \langle \psi^+_{\sigma_1}(\bar{r}_1) \psi_{\sigma_1}(\bar{r}_1) \rangle \langle \psi^+_{\sigma_2}(\bar{r}_2) \psi_{\sigma_2}(\bar{r}_2) \rangle$ = Hartree
$- \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 d^3 r_2 \frac{e^2}{4\pi\epsilon_0 |\bar{r}_1 - \bar{r}_2|} \langle \psi^+_{\sigma_1}(\bar{r}_1) \psi_{\sigma_2}(\bar{r}_2) \rangle \langle \psi^+_{\sigma_2}(\bar{r}_2) \psi_{\sigma_1}(\bar{r}_1) \rangle$ = Fock

$$\langle \hat{V}_{el\text{-}el} \rangle = \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 \, d^3 r_2 \, \frac{e^2}{4\pi \epsilon_0 |\bar{r}_1 - \bar{r}_2|} \left\langle \psi^{+}_{\sigma_1}(\bar{r}_1) \, \psi^{+}_{\sigma_2}(\bar{r}_2) \, \psi_{\sigma_2}(\bar{r}_2) \, \psi_{\sigma_1}(\bar{r}_1) \right\rangle$$

$$= \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 \, d^3 r_2 \, \frac{e^2}{4\pi \epsilon_0 |\bar{r}_1 - \bar{r}_2|} \left\langle \psi^{+}_{\sigma_1}(\bar{r}_1) \, \psi_{\sigma_1}(\bar{r}_1) \right\rangle \left\langle \psi^{+}_{\sigma_2}(\bar{r}_2) \, \psi_{\sigma_2}(\bar{r}_2) \right\rangle = \text{Hartree}$$

$$- \frac{1}{2} \sum_{\sigma_1 \sigma_2} \int d^3 r_1 \, d^3 r_2 \, \frac{e^2}{4\pi \epsilon_0 |\bar{r}_1 - \bar{r}_2|} \left\langle \psi^{+}_{\sigma_1}(\bar{r}_1) \, \psi_{\sigma_2}(\bar{r}_2) \right\rangle \left\langle \psi^{+}_{\sigma_2}(\bar{r}_2) \, \psi_{\sigma_1}(\bar{r}_1) \right\rangle = \text{Fock}$$

ree

ock

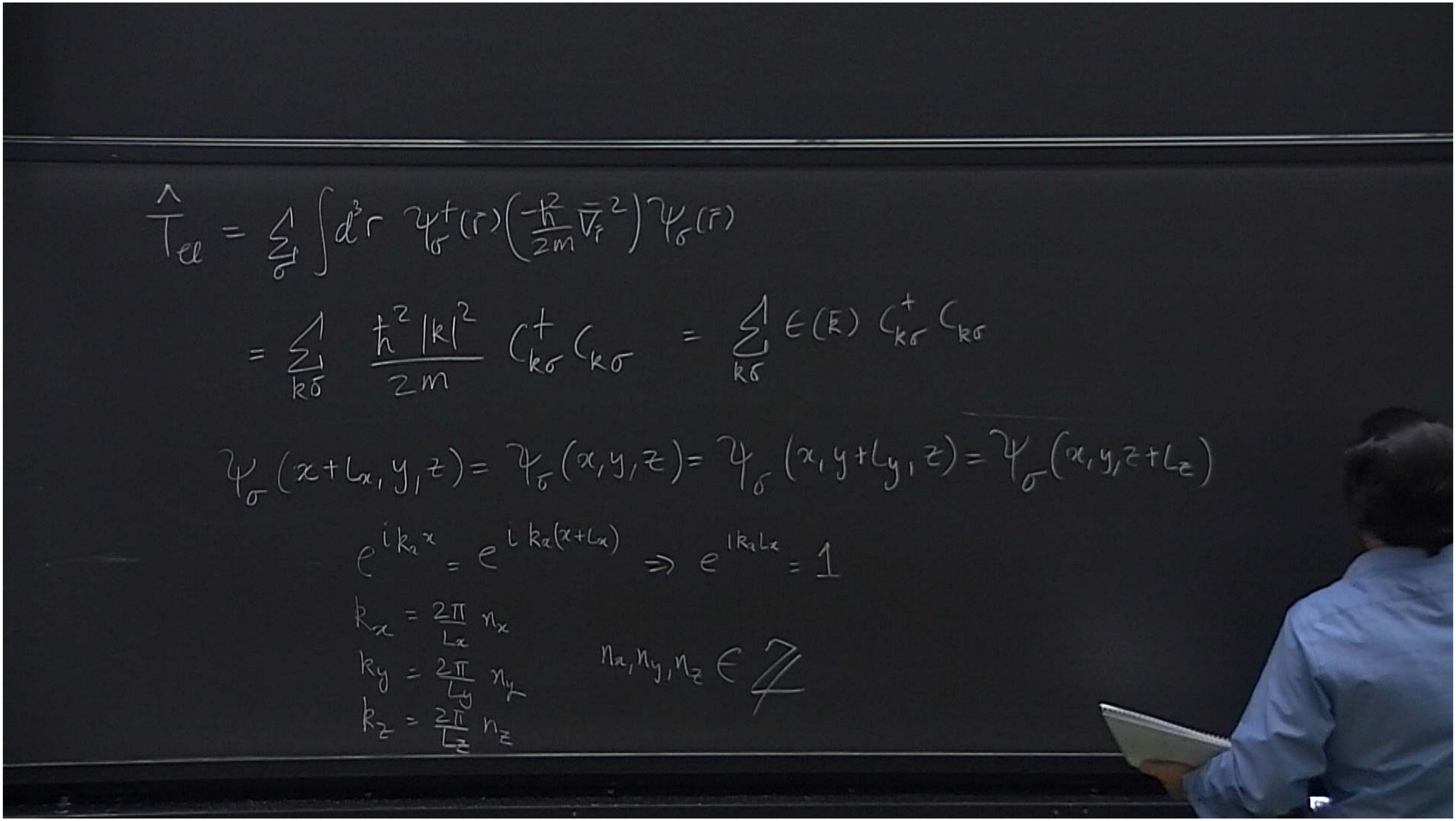
$$\langle \hat{V}_{el\text{-}el,\,Hartree} \rangle = \frac{\Omega}{2} \frac{e^2 \rho_{el}^2}{4\pi\epsilon_0} \int d^3R \, \frac{1}{|R|}$$

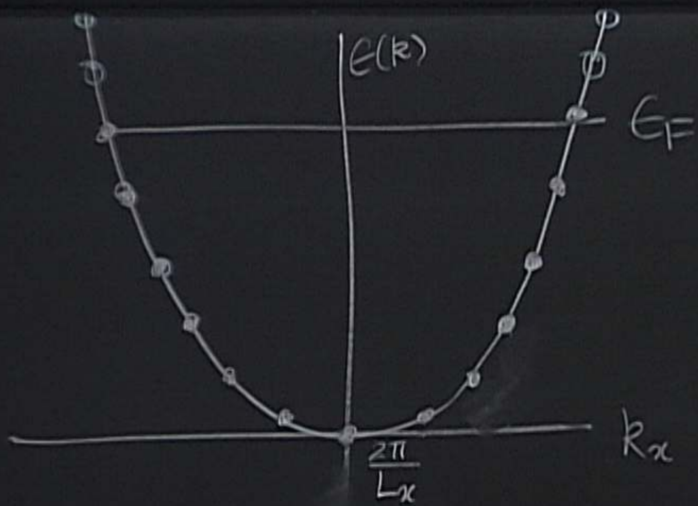
diverges as $|R| \to 0$

$$\hat{V}_{ion\text{-}ion} + \langle \hat{V}_{el\text{-}ion} \rangle + \langle \hat{V}_{el\text{-}el,\,Hartree} \rangle$$

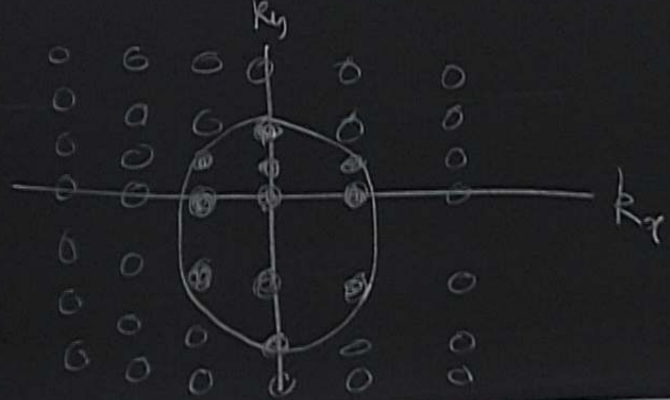
$$= \frac{\Omega}{2(4\pi\epsilon_0)} \left[(Ze)^2 \rho_{ion}^2 - 2(Ze^2)\rho_{ion}\rho_{el} + e^2 \rho_{el} \right] \int d^3R \, \frac{1}{|R|}$$

$$\rho_{el} = Z \rho_{ion}$$


$\hat{T}_{el} = \sum_{\sigma} \int d^3r \, \psi^{\dagger}_{\sigma}(\bar{r}) \left(\frac{-\hbar^2}{2m} \bar{\nabla}_r^{\,2} \right) \psi_{\sigma}(\bar{r})$
$= \sum_{k\sigma} \frac{\hbar^2 |k|^2}{2m} c^{\dagger}_{k\sigma} c_{k\sigma} = \sum_{k\sigma} \epsilon(\bar{k}) \, c^{\dagger}_{k\sigma} c_{k\sigma}$
$\psi_{\sigma}(x+L_x, y, z) = \psi_{\sigma}(x,y,z) = \psi_{\sigma}(x, y+L_y, z) = \psi_{\sigma}(x, y, z+L_z)$
$e^{ik_x x} = e^{ik_x(x+L_x)} \Rightarrow e^{ik_x L_x} = 1$
$k_x = \frac{2\pi}{L_x} n_x$
$k_y = \frac{2\pi}{L_y} n_y$
$k_z = \frac{2\pi}{L_z} n_z$
$n_x, n_y, n_z \in \mathbb{Z}$



Volume per state in k-space $= \frac{(2\pi)^3}{L_x L_y L_z} = \frac{(2\pi)^3}{\Omega}$



$$\frac{(2\pi)^3}{\Omega}$$

Fermi sphere (radius k_F)

$$|0\rangle = \prod_{|\bar{k}|<k_F} c^\dagger_{\bar{k}\uparrow}\, c^\dagger_{\bar{k}\downarrow}\, |\text{vacuum}\rangle$$

Fermi wavelength $\lambda_F = \dfrac{2\pi}{k_F}$

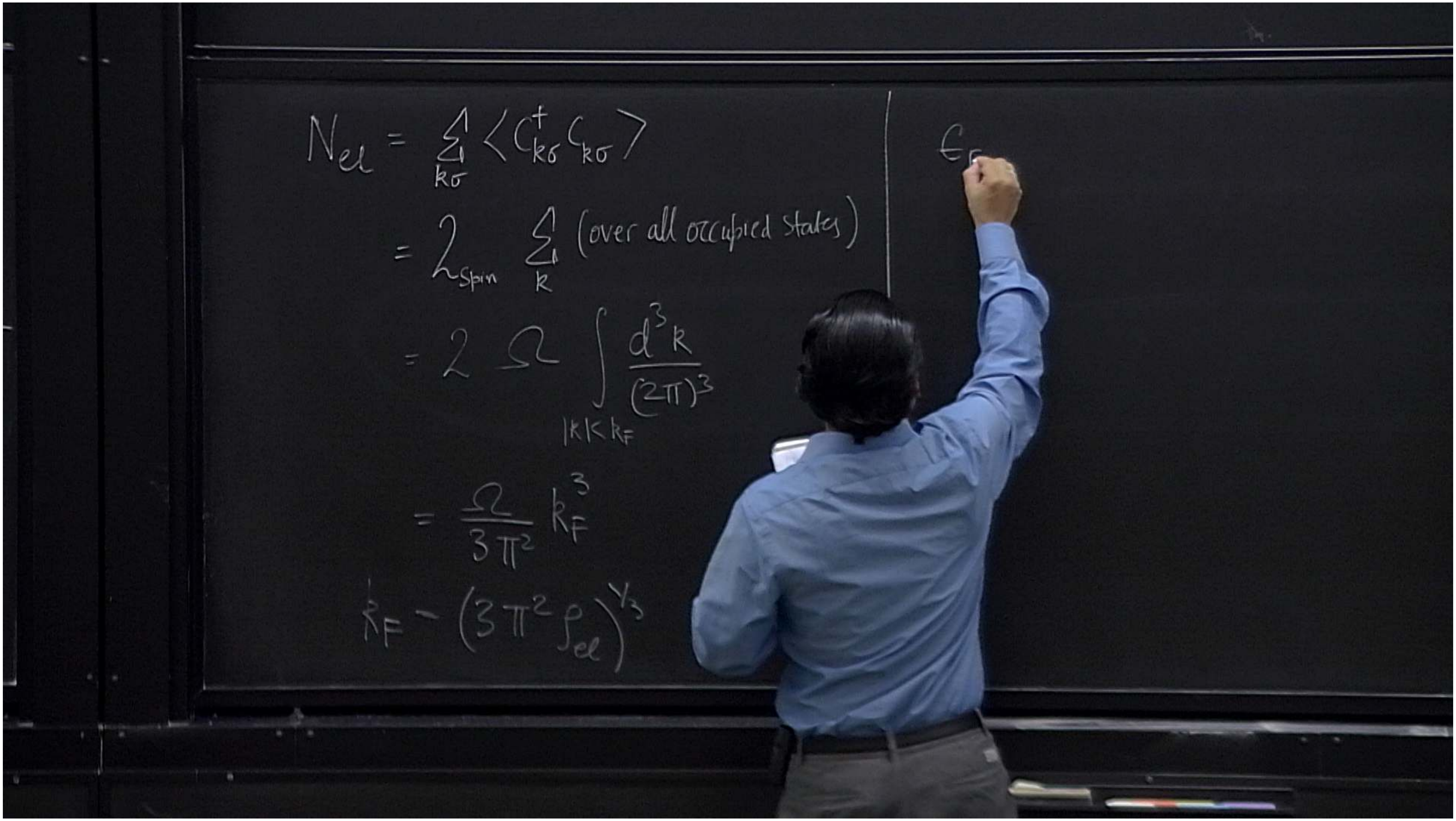
Fermi velocity $v_F = \dfrac{1}{\hbar}\dfrac{\partial \epsilon(k)}{\partial k}\Big|_{k_F} = \dfrac{\hbar k_F}{m}$

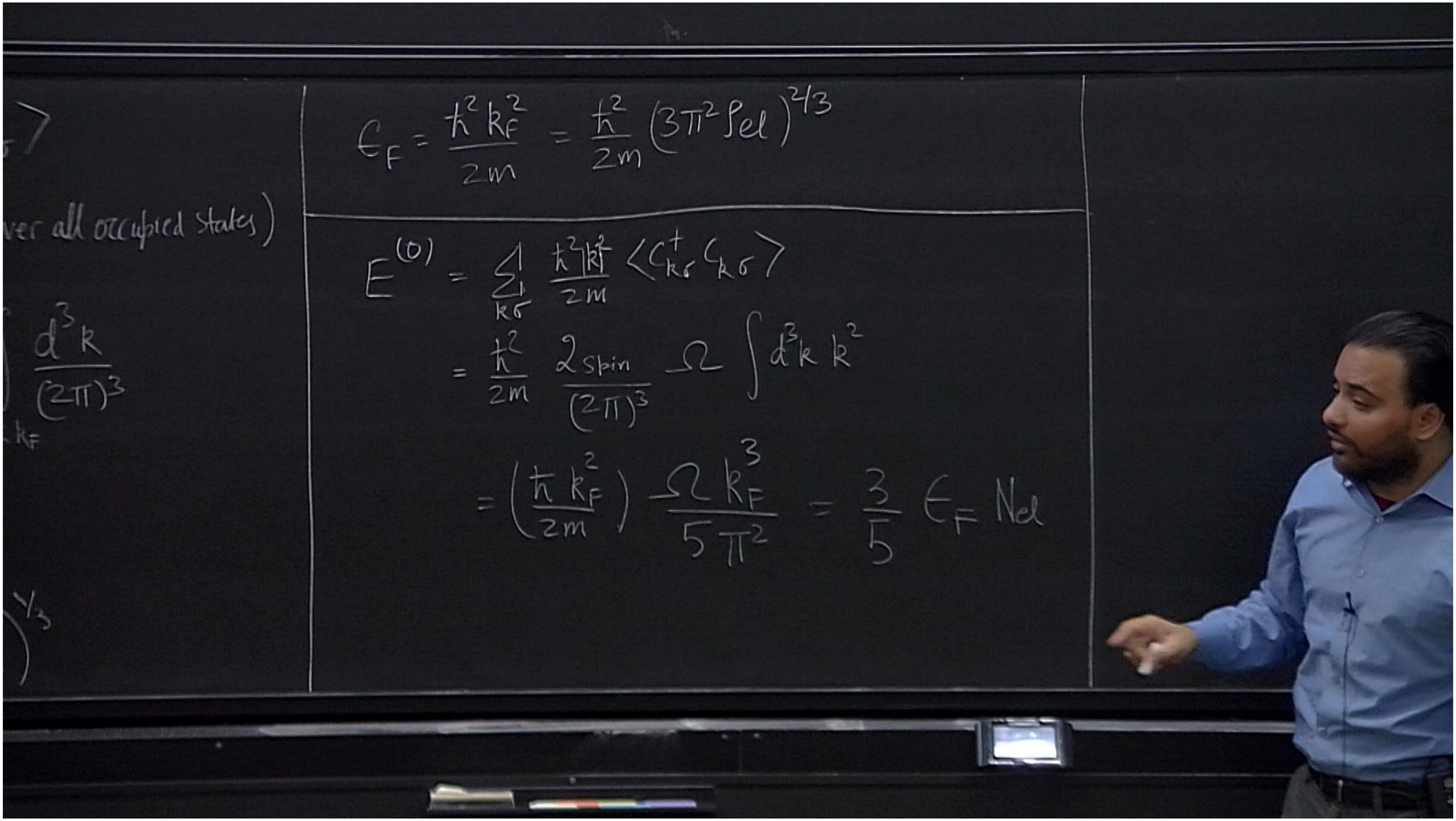
$$N_{el} = \sum_{k\sigma} \langle c^{\dagger}_{k\sigma} c_{k\sigma} \rangle$$

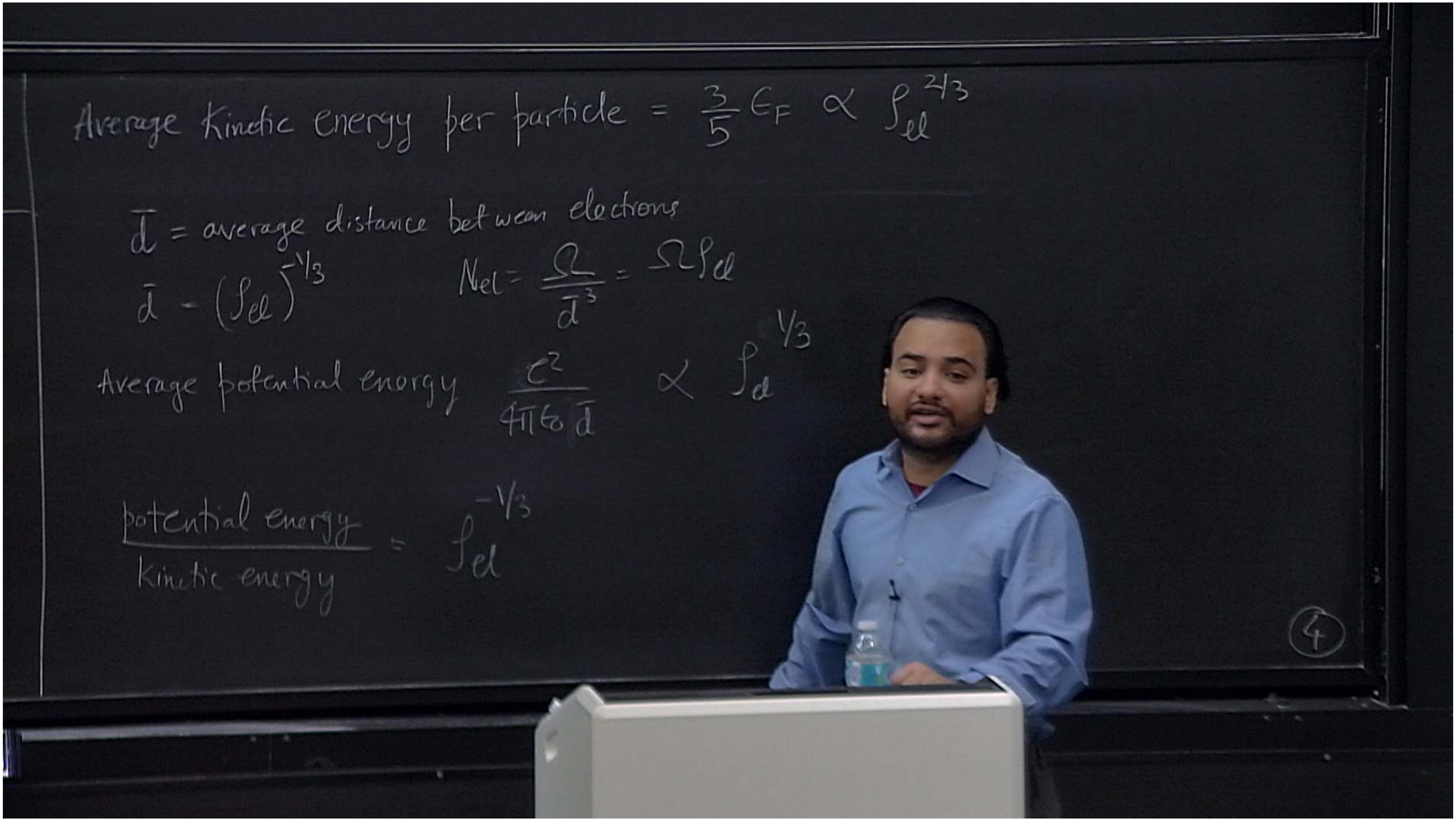
$$= 2_{\text{spin}} \sum_{k} \text{(over all occupied states)}$$

$$= 2\,\Omega \int_{|k|<k_F} \frac{d^3k}{(2\pi)^3}$$

$$= \frac{\Omega}{3\pi^2} k_F^3$$


$N_{el} = \sum_{k\sigma} \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle$
$= 2_{\text{spin}} \sum_{k}$ (over all occupied states)
$= 2\, \Omega \int_{|k|<k_F} \frac{d^3k}{(2\pi)^3}$
$= \frac{\Omega}{3\pi^2} k_F^3$
$k_F = (3\pi^2 \rho_{el})^{1/3}$
ϵ_F


ver all occupied states)
$\frac{d^3k}{(2\pi)^3}$
$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2 \rho_{el})^{2/3}$
$E^{(0)} = \sum_{k\sigma} \frac{\hbar^2 |k|^2}{2m} \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle$
$= \frac{\hbar^2}{2m} \frac{2_{spin}}{(2\pi)^3} \Omega \int d^3k\, k^2$
$= \left(\frac{\hbar^2 k_F^2}{2m}\right) \frac{\Omega k_F^3}{5\pi^2} = \frac{3}{5} \epsilon_F N_{el}$


Average Kinetic energy per particle = $\frac{3}{5}\epsilon_F \propto \rho_{el}^{2/3}$
$\bar{d}$ = average distance between electrons
$\bar{d} \sim (\rho_{el})^{-1/3}$
$N_{el} = \frac{\Omega}{\bar{d}^3} = \Omega \rho_{el}$
Average potential energy $\frac{e^2}{4\pi\epsilon_0 \bar{d}} \propto \rho_{el}^{1/3}$
$\frac{\text{potential energy}}{\text{Kinetic energy}} = \rho_{el}^{-1/3}$
4

$$k_y = \frac{2\pi}{L_y} n_y \qquad n_x, n_y, n_z \in \mathbb{Z}$$

$$k_z = \frac{2\pi}{L_z} n_z$$

Density of States $\rho(\epsilon)$

# of states between ϵ and $\epsilon + d\epsilon$

$$\rho(\epsilon) = \frac{dn}{d\epsilon} \qquad n = \frac{\text{Total Number of States}}{\Omega}$$

$$N = 2_{\text{spin}} \frac{\text{Volume in k-space}}{\text{Volume per state}} = 2 \frac{\frac{4}{3}\pi k_F^3}{\frac{(2\pi)^3}{\Omega}} = \frac{\Omega}{3\pi^2} k_F^3$$

$\epsilon_F = \hbar$

$$k_y = \frac{2\pi}{L_y} n_y \qquad n_x, n_y, n_z \in \mathbb{Z}$$

$$k_z = \frac{2\pi}{L_z} n_z$$

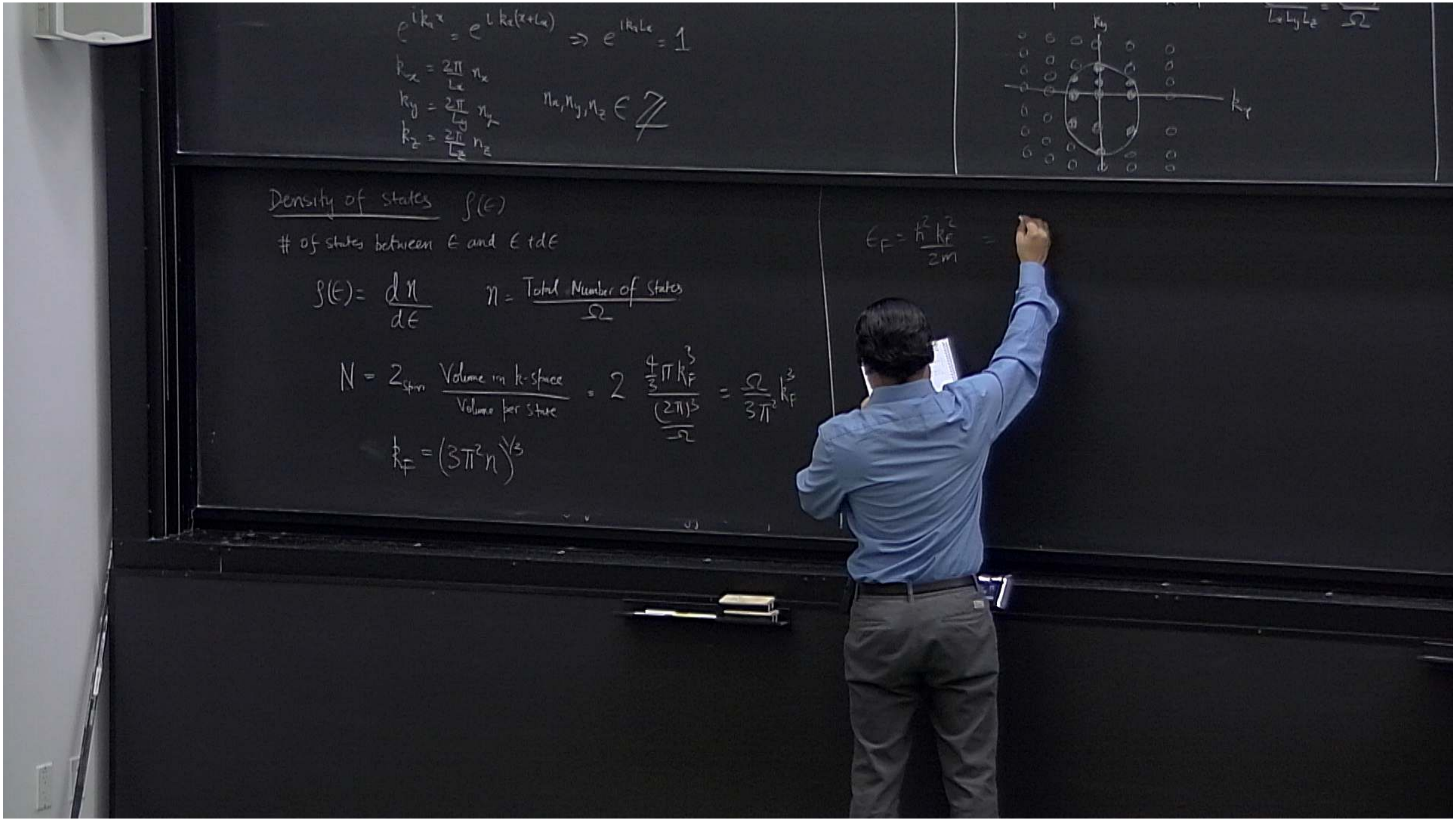
Density of States $\rho(\epsilon)$

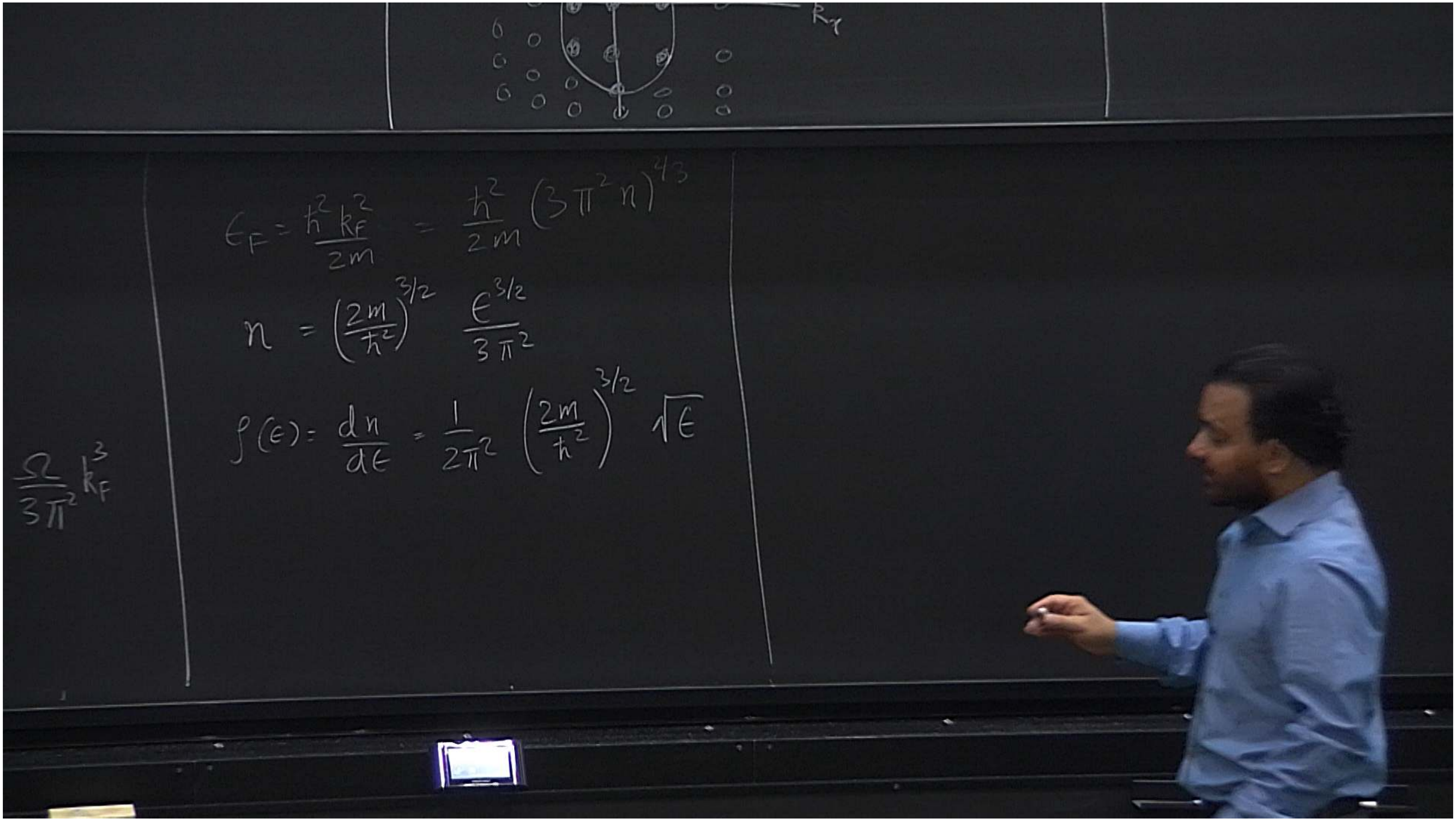
of states between ϵ and $\epsilon + d\epsilon$

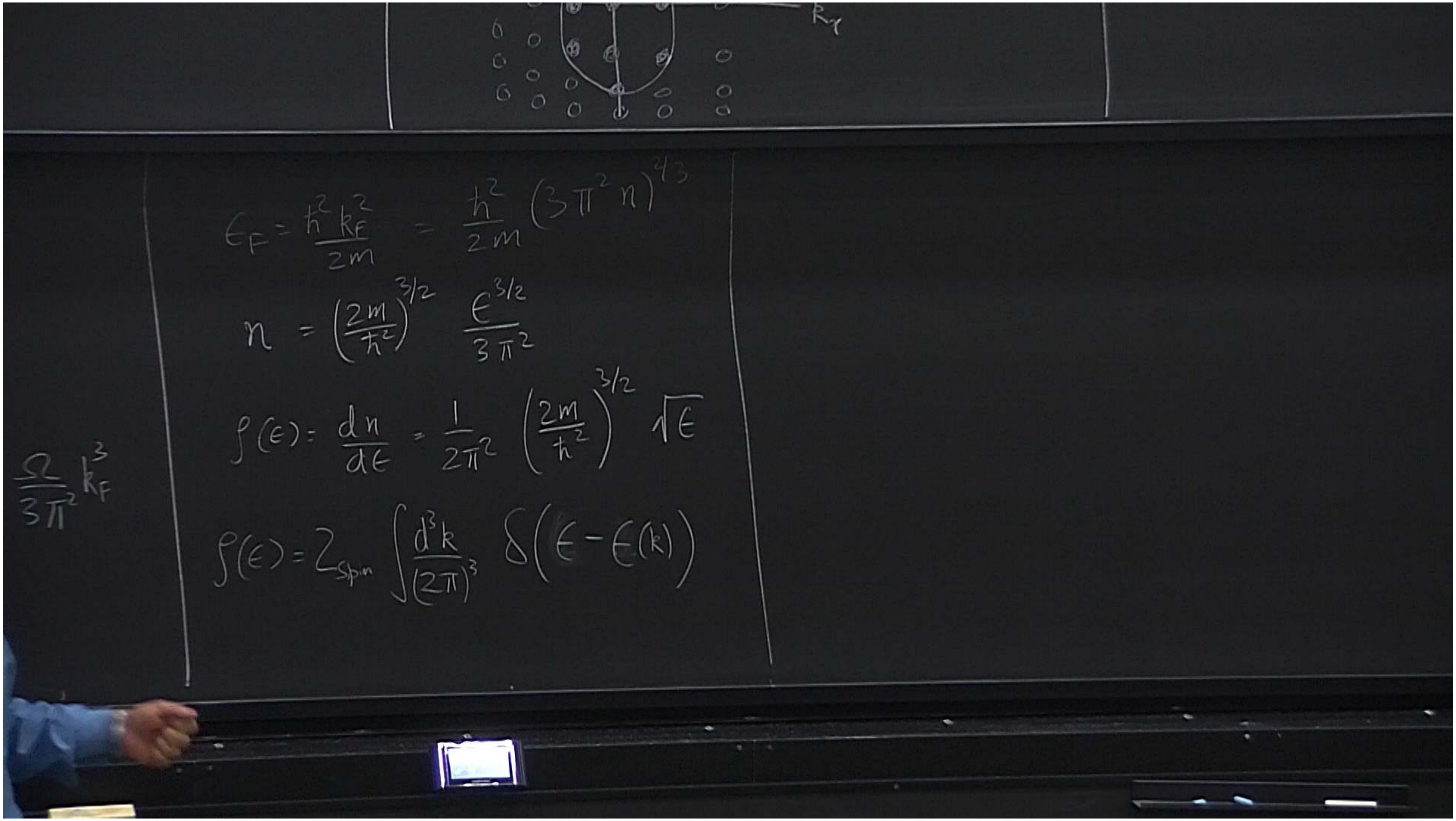
$$\rho(\epsilon) = \frac{dn}{d\epsilon} \qquad n = \frac{\text{Total Number of States}}{\Omega}$$

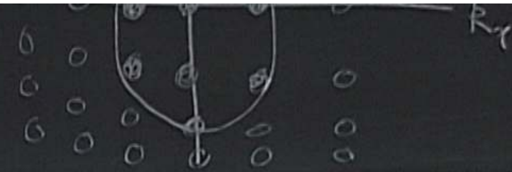
$$N = 2_{\text{spin}} \frac{\text{Volume in k-space}}{\text{Volume per state}} = 2 \frac{\frac{4}{3}\pi k_F^3}{\frac{(2\pi)^3}{\Omega}} = \frac{\Omega}{3\pi^2} k_F^3$$

$$k_F = (3\pi^2 n)^{1/3}$$


Density of states ρ(ε)
# of states between ε and ε+dε
ρ(ε) = dn/dε
n = Total Number of States / Ω
N = 2spin Volume in k-space / Volume per state = 2 (4/3 π k_F^3)/((2π)^3/Ω) = Ω/(3π^2) k_F^3
k_F = (3π^2 n)^(1/3)
ε_F = ħ^2 k_F^2 / 2m
k_x = 2π/L_x n_x
k_y = 2π/L_y n_y
k_z = 2π/L_z n_z
n_x, n_y, n_z ∈ Z


$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$
$n = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\epsilon^{3/2}}{3\pi^2}$
$\rho(\epsilon) = \frac{dn}{d\epsilon} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}$
$\frac{\Omega}{3\pi^2}k_F^3$


k_y
$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$
$n = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\epsilon^{3/2}}{3\pi^2}$
$\rho(\epsilon) = \frac{dn}{d\epsilon} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}$
$\frac{\Omega}{3\pi^2} k_F^3$
$\rho(\epsilon) = \sum_{spin} \int \frac{d^3k}{(2\pi)^3} \delta(\epsilon - \epsilon(k))$



$$= \frac{\Omega}{3\pi^2} k_F^3$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

$$n = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\epsilon^{3/2}}{3\pi^2}$$

$$\rho(\epsilon) = \frac{dn}{d\epsilon} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}$$

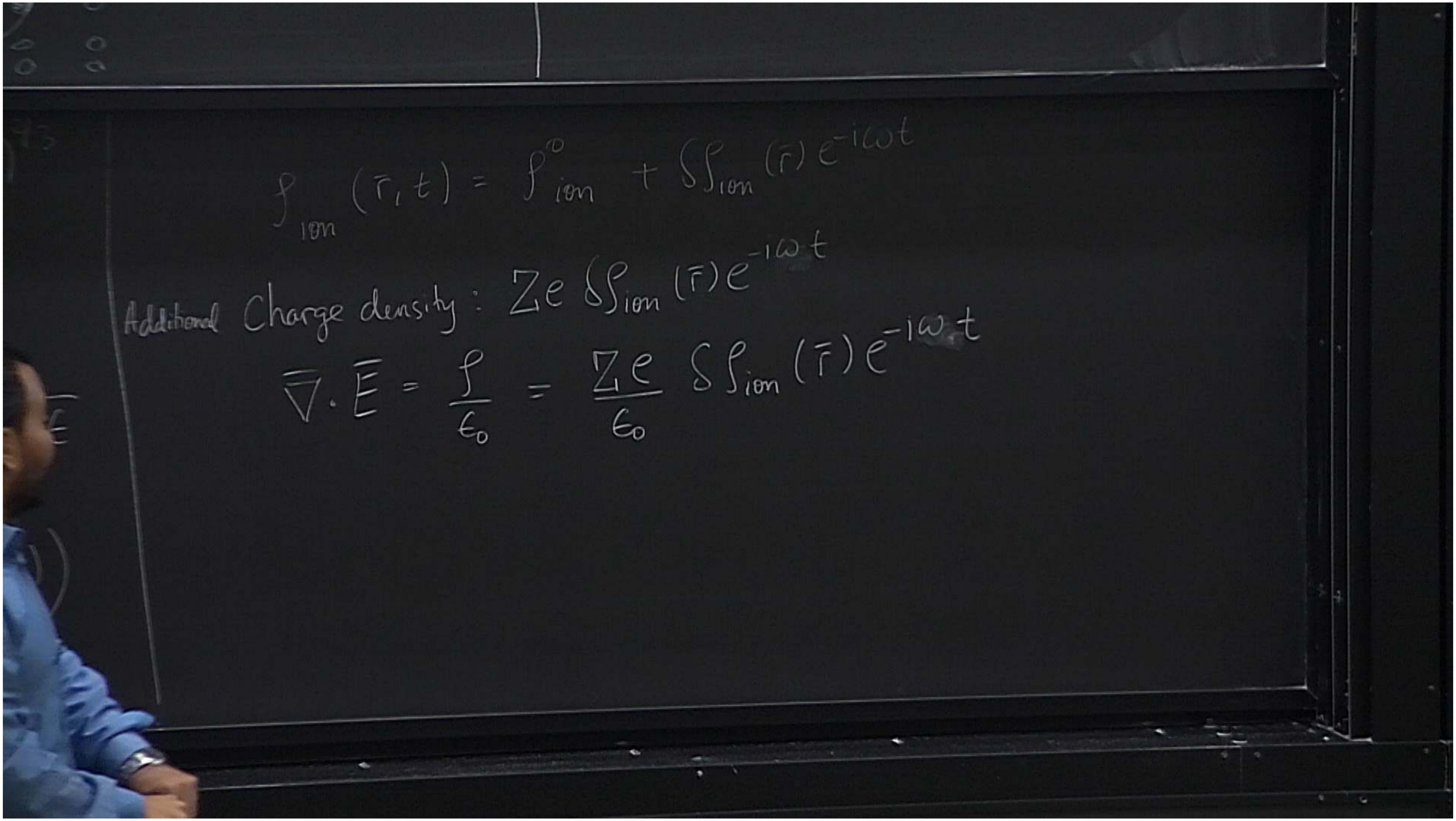
$$\rho(\epsilon) = \sum_{\text{spin}} \int \frac{d^3k}{(2\pi)^3}\, \delta\left(\epsilon - \epsilon(k)\right)$$

$$= \sum_{\text{spin}} \int_{S(\epsilon)} \frac{dS}{(2\pi)^3} \frac{1}{\left|\nabla_k \epsilon(k)\right|}$$

$$\rho_{ion}(\bar{r},t) = \rho^{0}_{ion} + \delta\rho_{ion}(\bar{r})\, e^{-i\Omega t}$$

Additional Charge density: $Ze\,\delta\rho_{ion}(\bar{r})\,e^{-i\Omega t}$

$$\bar{\nabla}\cdot\bar{E} = \frac{\rho}{\epsilon_0} = \frac{Ze}{\epsilon_0}\,\delta\rho_{ion}(\bar{r})\,e^{-i\Omega t}$$


$\rho_{ion}(\bar{r},t) = \rho^0_{ion} + \delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$
Additional Charge density: $Ze\,\delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$
$\bar{\nabla}\cdot\bar{E} = \frac{\rho}{\epsilon_0} = \frac{Ze}{\epsilon_0}\,\delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$

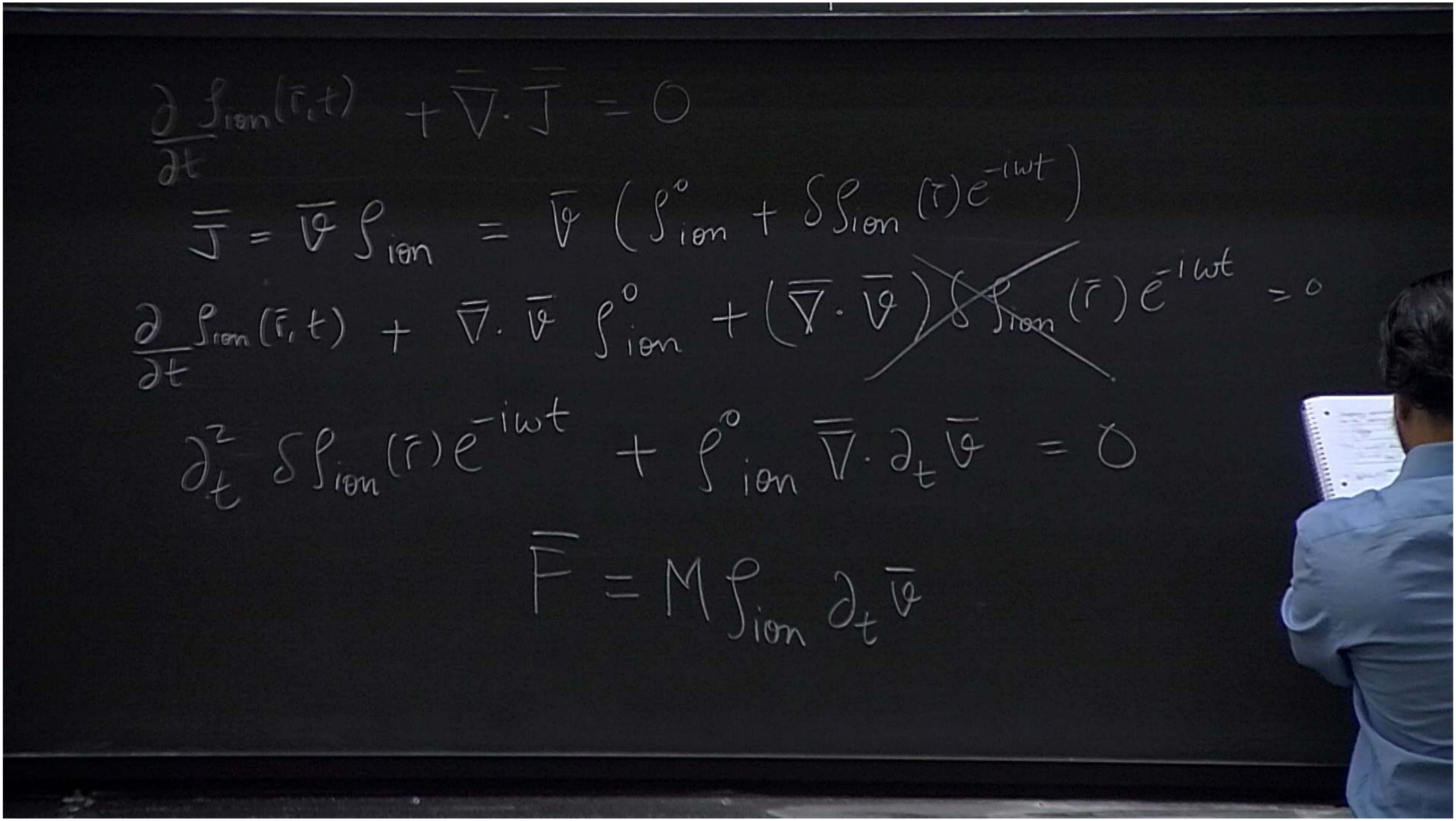
$$\rho_{ion}(\bar{r}, t) = \rho^0_{ion} + \delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$$

Additional Charge density: $Ze\,\delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$

$$\bar{\nabla}\cdot\bar{E} = \frac{\rho}{\epsilon_0} = \frac{Ze}{\epsilon_0}\,\delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$$

$$\bar{F} = \left(Ze\,\rho^0_{ion}\right)\bar{E}$$

$$\bar{\nabla}\cdot\bar{F} = \frac{Z^2 e^2 \rho^0_{ion}}{\epsilon_0}\,\delta\rho_{ion}(\bar{r})\, e^{-i\omega t}$$

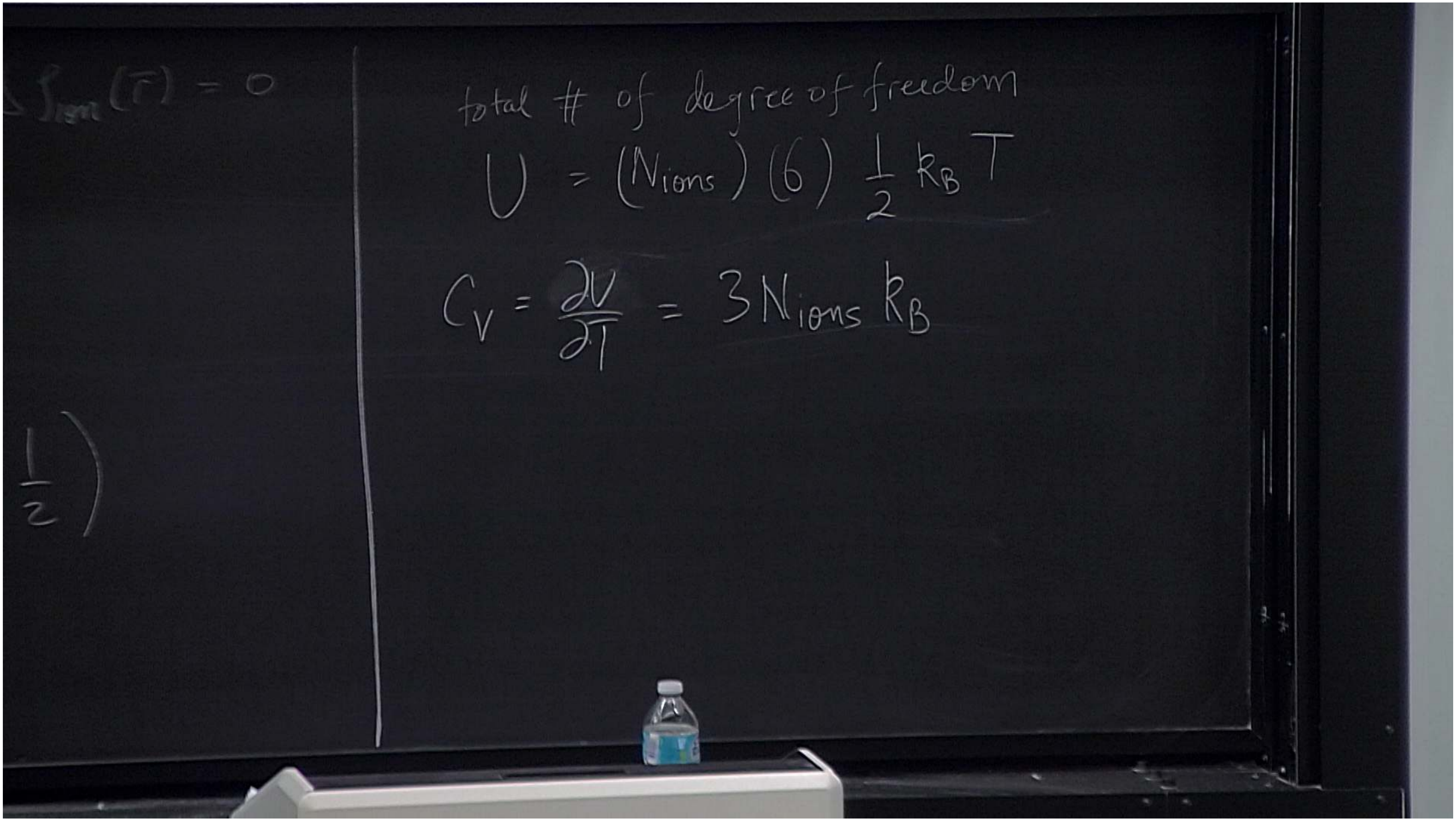


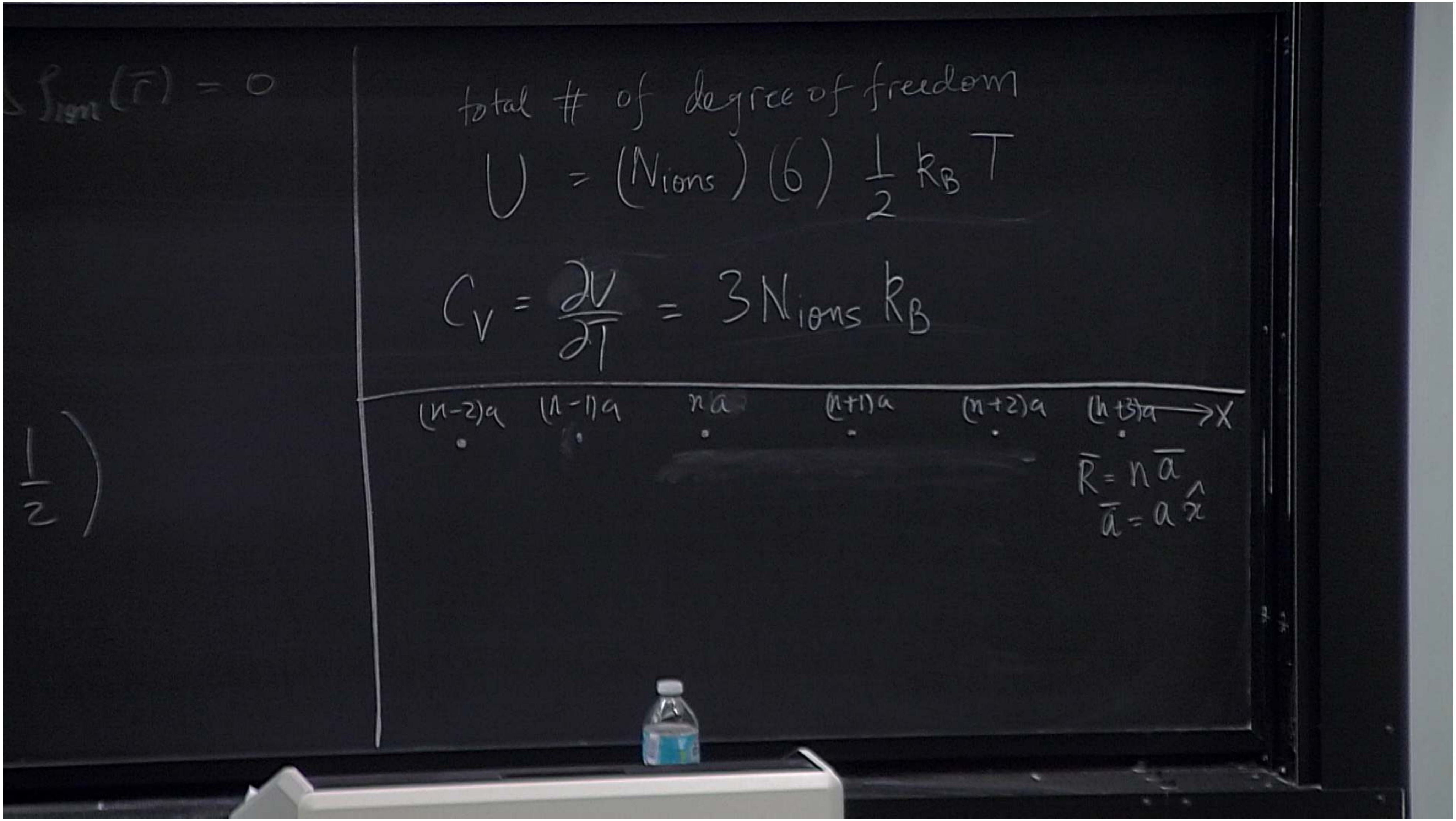
$\frac{\partial \rho_{ion}(\bar{r},t)}{\partial t} + \bar{\nabla}\cdot\bar{J} = 0$
$\bar{J} = \bar{v}\rho_{ion} = \bar{v}\left(\rho^{0}_{ion} + \delta\rho_{ion}(\bar{r})e^{-i\omega t}\right)$
$\frac{\partial \rho_{ion}(\bar{r},t)}{\partial t} + \bar{\nabla}\cdot\bar{v}\,\rho^{0}_{ion} + \cancel{(\bar{\nabla}\cdot\bar{v})\delta\rho_{ion}}(\bar{r})e^{-i\omega t} = 0$
$\partial_t^2\,\delta\rho_{ion}(\bar{r})e^{-i\omega t} + \rho^{0}_{ion}\,\bar{\nabla}\cdot\partial_t\bar{v} = 0$
$\bar{F} = M\rho_{ion}\,\partial_t\bar{v}$

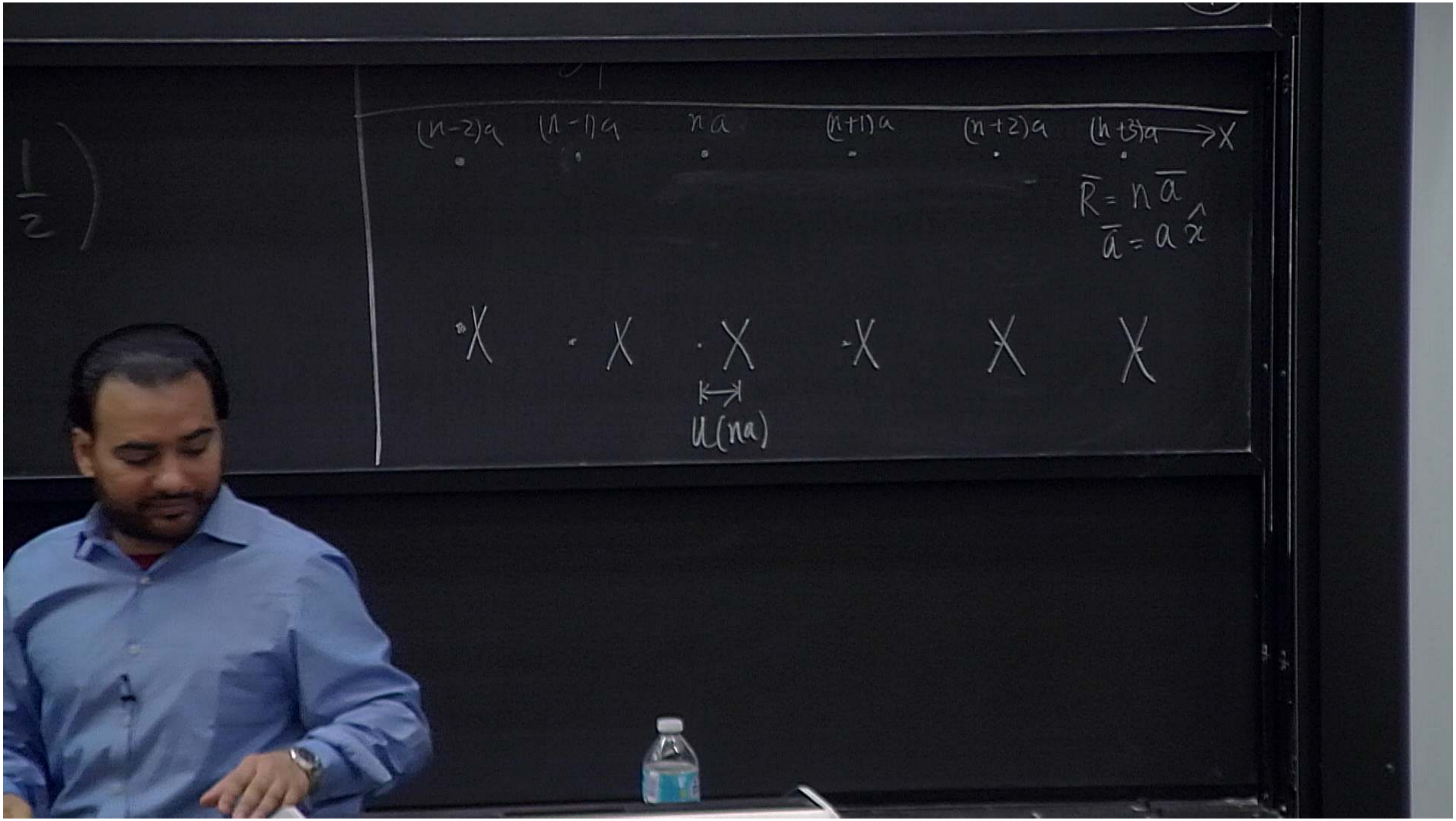
$$-\omega^2 \, \delta\rho_{ion}(\bar{r}) + \frac{1}{M} \frac{Z_i^2 e^2 \rho^0_{ion}}{\epsilon_0} \, \delta\rho_{ion}(\bar{r}) = 0$$

$$\omega = \sqrt{\frac{Z_i^2 e^2 \rho^0_{ion}}{\epsilon_0 M}}$$

$$H_{ph} = \sum_q \hbar \omega \left(b_q^+ b_q + \frac{1}{2} \right)$$


total # of degree of freedom
$U = (N_{ions})(6)\frac{1}{2}k_B T$
$C_V = \frac{\partial U}{\partial T} = 3N_{ions}k_B$


$\rho_{ion}(\bar{r}) = 0$
total # of degree of freedom
$U = (N_{ions})(6)\frac{1}{2}k_B T$
$C_V = \frac{\partial U}{\partial T} = 3N_{ions}k_B$
$(n-2)a$
$(n-1)a$
na
$(n+1)a$
$(n+2)a$
$(n+3)a$
X
$\bar{R} = n\bar{a}$
$\bar{a} = a\hat{x}$
$\frac{1}{2})$


(n-2)a
(n-1)a
na
(n+1)a
(n+2)a
(n+3)a
X
R̄ = n ā
ā = a x̂
u(na)